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14. ABSTRACT
On May 10-11, 2010, leading scientists and engineers of the tribological community convened at a workshop sponsored by the Air Force Office of Scientific Research to explore and identify future areas of fundamental tribological research. The changing landscape of fundamental knowledge, the development of new experimental, simulation, and modeling tools, and the rapid emergence of new technologies relying upon advanced tribological performance together provided the impetus for the workshop. Workshop participants are listed in Appendix A.
The workshop centered on the consideration, evaluation, and debate of issues currently limiting the advancement of our tribological understanding. The program was aided by the purposeful division of participants into groups of similar interests/expertise followed by group wide discussion of recommendations. Throughout the workshop, topic groups were regularly varied in order to maximize the cross disciplinary exchange of concerns and ideas. The resulting discussions produced three categories of information. First, reflections on the present state of the research field produced a list of successful technological applications that would not be possible without the advanced understanding of tribology fundamentals we are currently afforded. Second, group deliberations produced a detailed list of approaches needed to advance the field and dependent technologies during the next decade.

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Fundamentals of Tribology Workshop

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Fundamentals of Tribology

An AFOSR Sponsored Workshop
Gainesville, FL
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Project Summary

On May 10-11, 2010, leading scientists and engineers of the tribological community convened at a workshop sponsored by the Air Force Office of Scientific Research to explore and identify future areas of fundamental tribological research. The changing landscape of fundamental knowledge, the development of new experimental, simulation, and modeling tools, and the rapid emergence of new technologies relying upon advanced tribological performance together provided the impetus for the workshop. Workshop participants are listed in Appendix A.

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- Computations or computational abilities
- Macroscopic measurements
- Nano-scale experiments
- Chemically specific tools
- Interfacial mechanics
- Future materials

Third, considerations of the approaches required to advance the field produced a short list of *Grand Challenges* presently facing this community and resting upon many of the specifics outlined in the previous section.

- *Reliable Mechanical Interfaces in Extreme Environments*
- *Frictionless and Wearless Energy Systems*
- *Biocompatible, Biomimetic, and Biotribological Interfaces*

Together, the list of specific research topics with the overarching challenges presently faced represents a recommendation for future funding and effort within the community. Many of the activities will entail cross-disciplinary activity and collaboration. As evidenced by past successes, advances in these areas promise to deliver tremendous technological impact as well as both significant energy and cost savings.

Present Technological Impact of Tribological Systems

Hard drive information storage technology

Hard disk technology involves the proximal "reading" and "writing" of bits of information at high speeds and densities. The increase in storage densities enjoyed over the past 3 decades have relied upon the development of atomically thin hard coats and equisite control over semi-mobile molecular layers of lubricants. These tribological solutions provide the protection against the loss of data and insure the longevity and reliability of all hard disk devices.

Ceramic bearing systems (main engines of NASA's Space Shuttle)

Tribological failure of bearings of the main engine early in the Space Shuttle program represented one of the most significant technical challenges to insuring the reliability and on-going safety of the shuttle. Materials and interfacial engineering research led to the development of silicon nitride ceramic ball bearings that provided years of successful mission critical performance. This development addressed the severe wear experienced at cryogenic temperatures through the introduction of novel solid-film lubrications schemes.

DLP technology (digital micromirror device)

The technology of digital light processing (DLP) at the heart of optical projection systems extensively employed today rests upon the solution to the tribological events occurring at the atomic level. The devices operate on the principle of light reflection from an array of microscopic mirrors that are switched between positions through electrical actuation. Adhesion and wear greatly limited the lifetime of devices before a vapor phase lubrication scheme was discovered.

Required Approaches

***Computations or computational abilities** most needed to advance our fundamental understanding of tribological phenomena include the following:*

- Introduction of continuum phase field modeling with respect to sliding interfaces will provide opportunities to follow the evolution of tribological materials as a function of shear-induced transformation.
- Development of Ashby maps describing tribological materials/interfaces in an effort to assimilate the growing body of computational and experimental data.
- Continued emphasis on potential development with respect to coverage of a greater range of materials and conditions will provide additional opportunities for linking to experimental findings and identifying important materials.
- Development of practices for publication reporting of computational limitations will provide example for community in need of addressing accuracy, precision, and the basis for relating simulation to experiment.
- Modeling of reactions under confined environments, at interfaces, is needed to address

the influence and activity of tribochemistry.

- Technique development is needed to enable arge scale electronic structure calculations of tribological interactions, serial vs. parallel processing, quantum dynamics (including vibrational properties), and multiscale modeling.
- Establishment of a fiducial material/interface for computation/simulation efforts will provide means of evaluating emerging computational capabilities and tribological theories.

*The **data and/or measurements at the macroscopic scale** most needed to advance our fundamental understanding of tribological phenomena include the following:*

- Development of experimental capabilities providing for the complete characterization of tribological systems (chemical composition, environment, surface roughness, operation conditions, etc) will provide the details required for a fundamental understanding of tribological interfaces; needed capabilities include but are not limited to *in situ* sensing, temperature measurement, and spectroscopy.
- Standardized measurements are needed to improve the fidelity of tribological measurements across the community; the further development of instrumentation dedicated to force measurement will also address this need.
- Characterization of wear events in terms of chemistry, morphology, size, stress, energy barriers needed to create, and structure (point and extended defects) will provide information required for energy and materials savings.
- Establishment of a fiducial material/interface will provide means of evaluating emerging theories, evaluating methodologies, and relating to nanoscale measurements.

*The **nanoscale experiments or developments** most needed to advance our fundamental understanding of tribological phenomena include the following:*

- Development of calibration, force, displacement, and probe standards at the nanometer scale will provide the means for delivering reproducibility of quantitative nanoscale measurements.
- Introduction of *in-situ*/coupled/synchronous measurement capabilities for the characterization of temperature, atomic/molecular composition and structure, and plastic deformation will augment existing measurements of force and provide means to fully describe tribological events at this scale.
- Exploration of measurements on relevant time scales (e.g. high shear rates) will enhance the relevance of nanoscale measurements to macroscopic events.
- Development of approaches for the quantitative determination of contact areas and local fluid film thickness will serve to better define the limits of operation, the relevance of nanoscopic measurements, and the specifications of tribological simulations.
- Establishment of a fiducial material/interface will provide means of evaluating emerging theories, evaluating methodologies, and relating to simulations and macroscale measurements.

The ***chemically specific tools*** *most in need of development, utilization, and/or simulation include:*

- Emerging characterization tools entailing elements of both microscopy and spectroscopy (nanoIR, X-ray microtomography, MALDI TOF-MS, TOF-SIMS, magnetic resonance imaging) offer the opportunity for integration of shear force measurements and the evaluation of sub surface structure and composition.
- Detailed and interface specific chemical information is needed as input to models: atomic composition, atomic structure, molecular structure, distribution of chemical species.
- Experimental tribometry measurements will require the ability to characterize a system before, during, and after shear events in order to understand the evolution of interfacial properties.
- Chemically specific nanoscopic spatial probes are needed to identify the mechanistic pathways describing the evolution of tribological interfaces.
- Labeling/spectroscopic studies are needed for the study of biotribological interfaces as a result of their inherent molecular complexity.

The measurements, models, tools, or systems most in need of being addressed by the ***mechanics*** *community include:*

- Measurements of the intrinsic mechanical properties of nanoparticles will provide needed input to modeling efforts (e.g. scaling laws are needed to describe system pressure and shear at the nanometer scale).
- Advancement of detailed atomistic models is still required to describe systems exhibiting nonlinear energy dissipation (e.g. stick slip behavior).
- Development of active control systems, entailing the coupling of embedded actuators and sensors for the purpose of controlling interfacial friction and wear, will benefit many future technologies.
- Development of mechanical models of soft materials (polymers) will be required to allow their greater incorporation into tribological systems; viscoelastic models are needed to describe the deformation of polymers from initiation to fracture;
- Expansion of mechanical models to address complex biological materials is needed to describe the distribution of forces and influence of interfacial stress.
- Consideration of plasticity and adhesion (including chemical effects) will allow the advancement of the understanding of wear at the atomic and molecular scale.
- Time correlated measurements of environmental history and structural evolution will reveal mechanistic pathways of tribological responses (friction and wear).

The ***materials, interfaces, fluids, or lubricants*** *most in need of investigation include:*

- Applied Materials
  - Adaptive materials
  - Structurally engineered materials
  - Environmentally friendly/insensitive solid/liquid lubricants

Thermally stable interfaces (room temperature to 1000°C)
Wear resistant polymers
Nanomaterials and nanolubricants

- Archetypal materials (single crystals readily available except for bio/polymers)
  Gold, gold copper alloys (metallic)
  MgO, ZnO (ionic)
  $SrTiO_3$ (partially ionic)
  Graphite (covalent, lamellar)
  Diamond (network covalent)
  Bone/Hydroxyapatite
  PMMA/PTFE/Polyethylene/Polycarbonate/Polystyrene (polymeric)
- Model Biological Materials
  Single cell studies (e.g. E-coli)
  Biomaterials (e.g. implants that last > 15 years)
  Surface coatings/treatments which do not damage cells during sliding
  Surface coatings/treatments which *do* damage cells – to prevent fouling
- Environmental Materials
  Water and hydrocarbons as third bodies
  Controllable friction (thermal, stress, chemical induced changes)
  Biologically compatible tribological interfaces
  Corrosion resistant tribological coatings
  Self-healing materials

Grand Challenges

#1 Reliable Mechanical Interfaces in Extreme Environments

Interfaces subject to loading, shearing, and sliding are ubiquitous in mechanical systems and devices, and many technologies are stalled due to the failure of such interfaces in extreme environments, including chemical, thermomechanical, electromagnetic, and radiative extremes. The ability to work in extreme environments offers extended operating ranges with improved performance in existing technologies, such as greatly increased efficiency and longevity in engines and turbines. In addition, the ability to operated under extreme environments will enable entirely new technologies, such as nanomechanical switches to replace transistors. The grand challenge is to develop novel materials and engineering designs to achieve desired tribological performance under these harsh conditions, which will reap economic, energy, and environmental benefits.

Impacted technologies:
- power generation
- space applications
- car engines (lightweight materials, higher temps)
- rail gun
- NEMS switches
- Microelectronics/MEMS

- Phased-array radar system

Extreme environments:
- temperature
- stress
- high velocity and strain rate
- chemically aggressive
- radiation
- electromagnetic
- longevity – long time scales
- particulates/contaminants (sand, ash)

#2 Frictionless and Wearless Energy Systems

Ultra high efficiency and long term durability of the country's power generation infrastructure requires technology that eliminates wear and minimizes friction of the moving assemblies. In addition, the efficiency of automotive and truck engines could be increased by 30% leading to a significant reduction in oil consumption and dependence on foreign oil. For example, current wind turbine capacity is currently limited by the tribological durability of gear box components within the rotor; in addition, lower friction assemblies would enable efficient operation at lesser wind velocities. While ultra low friction materials and extremely low wear rate materials exist for isolated situations, an extensive set of materials have not been developed appropriate for service environments. Meeting this grand challenge calls for fundamental studies of tribological behavior under high stress, variable loading, and realistic shear velocities, employing both computation and experimentation to develop input to the future mechanical design of frictionless and wearless energy systems. Furthermore, the benefits of such development can easily be seen to positively impact any mechanical system that involves components subjected to rolling, rotating, or sliding.

#3 Biocompatible, Biomimetic, and Biotribological Interfaces

Living systems are replete with biointerfaces, many of which are exposed to varying degrees of mechanical interaction. These interfaces successfully function within complex physiological environments with generally extended lifetimes, thus offering sophisticated models for future tribological designs. Furthermore, biotechnology often entails the introduction of a foreign material to the system, such as in the case of the contact lens or biomedical implant, generating unique, non-native interfaces each required to function in a manner consistent with its specific biological environment. The grand challenge is thus to understand the function and performance of sliding interfaces within living systems at the level of specific biomolecular entities and their unique properties (viscoelasticity, poroelasticity, interfacial adhesion). In turn, this understanding will enable the development of future tribofunctional biomaterials matching the performance of the native interface found within living systems, the development of biomimetic interfaces allowing for extended operation under aqueous environments, and the discovery of stress/shear modulated methods of cellular communication within living systems.

Appendix A

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